Problem sheet 5: Mechanical properties, Dielectric properties **8.11.2023**

5.1. Equation of state (5 P)

(a) Derive Murnaghan equation of state assuming linear pressure dependence of the bulk modulus, $B(p) = B_0 + B_0' \, p$.

(b) Use experimental lattice parameters of α-quartz (SiO_2, space group $P3_12$ or $P3_22$) to determine B_0 and B_0'.

Hint: get lattice parameters from the Crystallography Open Database. If you find it difficult to solve non-linear equations or fit the non-linear function, choose $B_0' = 6.0$ and determine B_0 only.

(c) Calculate the shift in the angular positions (2θ) of the 100 and 101 reflections of α-quartz between 0 GPa and ~ 5 GPa. Choose $\lambda = 0.4$ Å as the typical wavelength in high-pressure XRD experiments.

Hint: Use the result from the problem 3.2 or VESTA.

5.2. Elastic constants and energies (4 P)

(a) Express the bulk modulus of a cubic crystal via its elastic constants. Determine the bulk modulus of copper using $C_{11} = 168$ GPa and $C_{12} = 122$ GPa.

(b) Elastic energy (per volume) is related to the product of σ and ε and can be written as

$$\mathcal{E} = \frac{1}{2} \sum_{\alpha,\beta} \varepsilon_\alpha C_{\alpha\beta} \varepsilon_\beta$$

where α and β are indices of the elastic constants tensor $C_{\alpha\beta}$ $(1 \ldots 6)$. Calculate elastic energy for the compressive strain of 1 %, which is caused by a uniaxial stress applied to the copper crystal along its [100] direction. Express the result in meV per atom. Use Poisson's ratio $\nu = 0.35$.

5.3. Microwave heating (5 P)

In the Debye model of relaxation, the permittivity $\varepsilon = \varepsilon' + i\varepsilon''$ due to permanent dipoles is given by

$$\varepsilon(\omega) = \varepsilon_\infty + \frac{\varepsilon_{\text{st}} - \varepsilon_\infty}{1 - i\omega\tau}$$

where ε_{st} is the static permittivity, ε_∞ is the permittivity in the high-frequency limit (was taken as 1 in the lecture), and τ is the relaxation time.

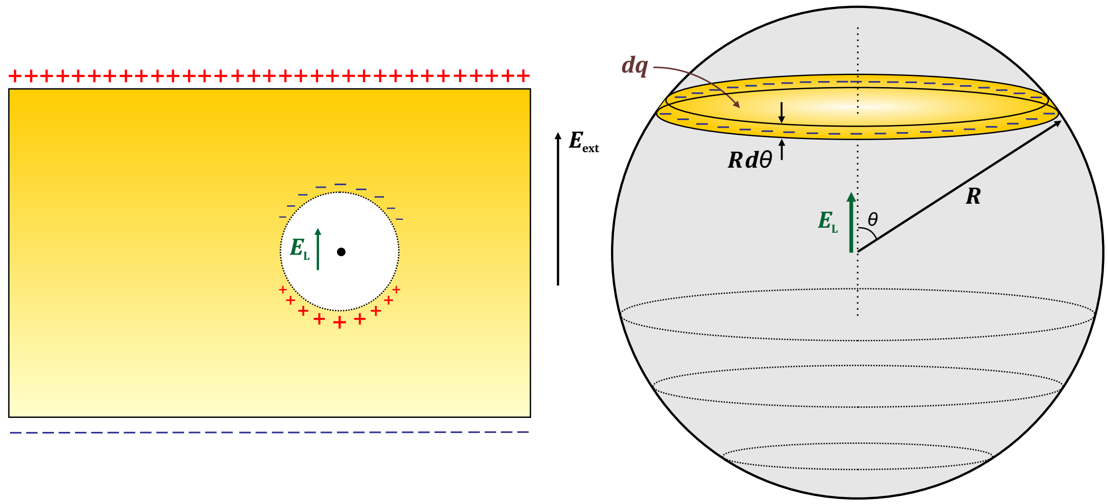
(a) Show that the dependence of ε'' on ε' (Cole-Cole plot) has the shape of a semi-circle. Determine the position of its center and the radius.

(b) At 20 °C, water has $\varepsilon_{\text{st}} = 80$, $\varepsilon_\infty = 2$, and the maximum dielectric loss at the frequency $\nu = 17$ GHz. Determine τ.

(c) Determine the loss tangent at 2.4 GHz, the frequency of the standard microwave oven.

(d) A typical liquor (40% alcohol) has $\varepsilon_{\text{st}} = 62$, $\varepsilon_\infty = 1.6$, and $\tau = 24$ ps. Which liquid, water or liquor, will be heated faster in the microwave oven?

Be careful if you choose to check this experimentally



5.4. Lorentz field and polarizability (6 P)

Polarizability is defined with respect to the local electric field, $\mathbf{E}_{\text{local}} = \mathbf{E}_{\text{ext}} + \mathbf{E}_L$, that includes Lorentz field $\mathbf{E}_L$ caused by induced charges in the vicinity of an atom/molecule. Show that $\mathbf{E}_L = \mathbf{P}/3\varepsilon_0$ where $\mathbf{P}$ is electric polarization, and use this result to derive the Clausius-Mossotti relation and determine polarizabilities.

(a) Consider a small sphere that is cut out in the middle of the sample. Positive and negative charges will occur on different sides of this sphere as the sample is polarized. Choose a slice with the thickness of $R\,d\theta$ and calculate its charge dq using $P(\theta) = -P\cos\theta$ (negative charge at the top, positive charge at the bottom, no charge at the equator). Remember that polarization is charge per area.

(b) Calculate the electric field dE_L created by this charge dq in the center of the sphere. Then integrate this electric field over θ to obtain $E_L = P/3\varepsilon_0$.

(c) Derive the Clausius-Mossotti relation between permittivity ε and polarizability α,

$$\frac{\varepsilon - 1}{\varepsilon + 2} = \frac{n_d\,\alpha}{3\varepsilon_0}$$

(d) Use static permittivities of chlorine ($\varepsilon = 2.0$), bromine ($\varepsilon = 3.1$), and iodine ($\varepsilon = 11.0$) to determine polarizabilities of the corresponding molecules. Explain the trend in the melting points of these elements. Use the densities of $\rho = 1.47\,\text{g/cm}^3$, $3.12\,\text{g/cm}^3$, and $4.93\,\text{g/cm}^3$ for Cl_2, Br_2, and I_2, respectively. Express polarizability in CGS units by choosing $\varepsilon_0 = 1/(4\pi)$. Then α becomes comparable to an effective volume of the molecule.

Hint: parts (c) and (d) can be solved even you do not know how to complete (a) and (b).